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=> fil casreact
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FILE CONTENT:1840 - 28 Sep 2008 VOL 149 ISS 14

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************************************************************
*                                                          *
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*                                                          *
************************************************************

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=> d que l5
L3                STR
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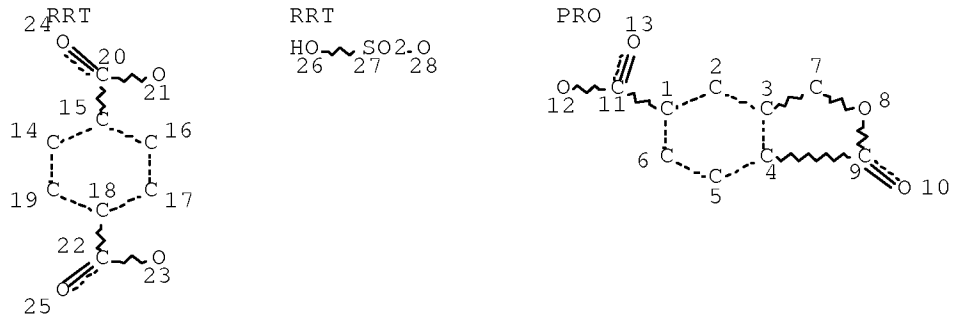


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  28

STEREO ATTRIBUTES: NONE
L5             8 SEA FILE=CASREACT SSS FUL L3 (    13 REACTIONS)
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=> fil cap
FILE 'CAPLUS' ENTERED AT 15:14:44 ON 29 SEP 2008
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FILE COVERS 1907 - 29 Sep 2008  VOL 149 ISS 14
FILE LAST UPDATED: 28 Sep 2008  (20080928/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
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http://www.cas.org/legal/infopolicy.html

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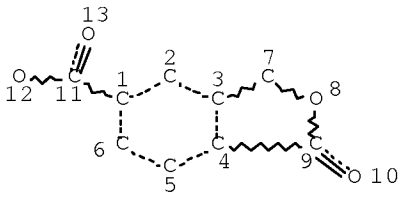


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
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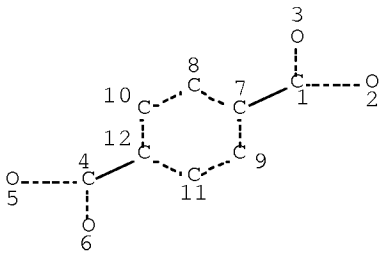

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STEREO ATTRIBUTES: NONE

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L16 29207 SEA FILE=REGISTRY ABB=ON PLU=ON (110-88-3/CRN OR 30525-89-4/CRN OR 50-00-0/CRN) OR L15
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L18 5714 SEA FILE=CAPLUS ABB=ON PLU=ON L8(L)PREP+NT/RL
L19 8 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L17
L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 OR 8014-95-7/CRN
L21 567 SEA FILE=CAPLUS ABB=ON PLU=ON L20(L)RACT+NT/RL
L22 3 SEA FILE=CAPLUS ABB=ON PLU=ON L19 AND L21
L23 3 SEA FILE=CAPLUS ABB=ON PLU=ON L21 AND L8 AND (L11 OR L16)
L24 8 SEA FILE=CAPLUS ABB=ON PLU=ON L19 OR L22 OR L23

=> dup rem l5 l24
FILE 'CASREACT' ENTERED AT 15:14:50 ON 29 SEP 2008
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PROCESSING COMPLETED FOR L5
PROCESSING COMPLETED FOR L24
L25 11 DUP REM L5 L24 (5 DUPLICATES REMOVED)
ANSWERS '1-8' FROM FILE CASREACT
ANSWERS '9-11' FROM FILE CAPLUS

=> d l25 ibib abs crd 1-8;d l25 ibib abs hitstr 9011

L25 ANSWER 1 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 147:52790 CASREACT Full-text

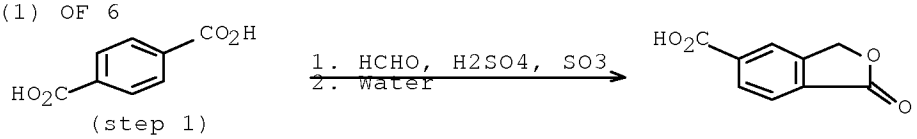
TITLE: Multi-step process for the preparation of 5-cyanophthalide from terephthalic acid and paraformaldehyde
INVENTOR(S): Mahavir, Arora Sunil
PATENT ASSIGNEE(S): Ipca Laboratories Limited, India
SOURCE: Indian Pat. Appl., 9pp.
CODEN: INXXBQ
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 2003MU01074	A	20050909	IN 2003-MU1074	20031016

PRIORITY APPLN. INFO.: IN 2003-MU1074 20031016

AB A multi-step process for the preparation of 5-cyanophthalide from terephthalic acid and paraformaldehyde is presented.

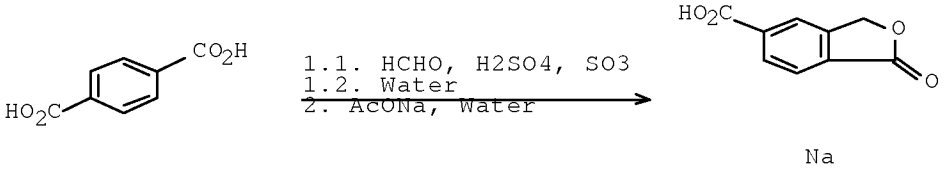
RX(1) OF 6



(step 1)

NOTE: paraformaldehyde used
CON: STAGE(1) room temperature -> 100 deg C; 3 hours; 2 hours, 110 - 120 deg C; 120 deg C -> room temperature
STAGE(2) cooled

RX(4) OF 6 - 2 STEPS



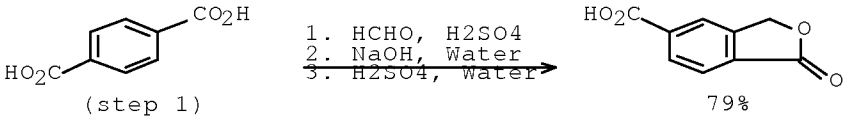
NOTE: 1) paraformaldehyde used
CON: STEP(1.1) room temperature -> 100 deg C; 3 hours; 2 hours, 110 - 120 deg C; 120 deg C -> room temperature
STEP(1.2) cooled
STEP(2) room temperature -> 80 deg C

L25 ANSWER 2 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 145:335870 CASREACT Full-text
TITLE: Synthesis of citalopram hydrobromide
AUTHOR(S): Wu, Qiuye; Liao, Hongli; Zhao, Huiqing; Ye, Guangming; Jin, Yongsheng
CORPORATE SOURCE: School of Pharmacy, Second Military Medical University, Shanghai, 200433, Peop. Rep. China
SOURCE: Zhongguo Yiyao Gongye Zazhi (2005), 36(1), 6-8
CODEN: ZYGZEA; ISSN: 1001-8255
PUBLISHER: Zhongguo Yiyao Gongye Zazhi Bianjibu
DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Citalopram hydrobromide [i.e., 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile monohydrobromide] was synthesized from terephthalic acid and paraformaldehyde by condensation to give 5-carboxyphthalanone, which subjected to condensation, amidation and dehydration to afford 5-cyanophthalanone followed by twice Grignard reaction, cyclization and then salification with an overall yield of 31%.

RX(2) OF 10



(step 1) 79%

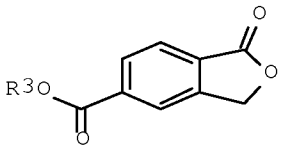
NOTE: paraformaldehyde used
CON: STAGE(1) room temperature -> 142 deg C; 5 hours, 142 deg C
STAGE(2) pH 7
STAGE(3) pH 2

L25 ANSWER 3 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 141:314145 CASREACT Full-text
TITLE: Preparation of 5-alkoxycarbonylphthtalides as intermediates for the preparation of citalopram and escitalopram
INVENTOR(S): Pittelkow, Thomas; Castellin, Andrea; Sbrogio, Federico; Dahlberg, Nielsen Poul; Zanon, Jacopo; Soegaard, Steen; Humble, Rikke Eva
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004083197	A2	20040930	WO 2004-DK177	20040317
WO 2004083197	A3	20041028		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2519629	A1	20040930	CA 2004-2519629	20040317
EP 1611118	A2	20060104	EP 2004-721125	20040317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1761659	A	20060419	CN 2004-80007510	20040317
IN 2005CN02322	A	20070302	IN 2005-CN2322	20050920

US 20080058536 A1 20080306 US 2007-550419 20070530
PRIORITY APPLN. INFO.: DK 2003-440 20030321
US 2003-456415P 20030321
WO 2004-DK177 20040317
OTHER SOURCE(S): MARPAT 141:314145

GI



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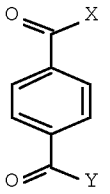
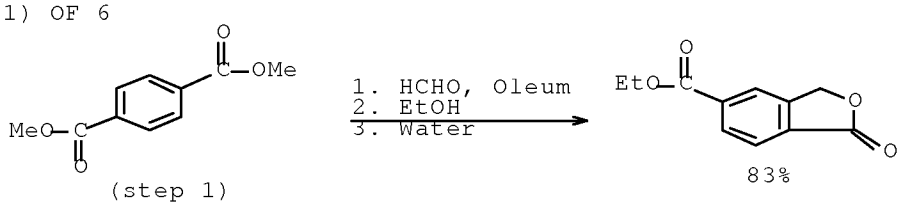


II

AB Methods for manufacture of 5-alkoxycarbonylphthtalides (I; R3 = C1-6 alkyl, Ph) are disclosed, which comprise (a) reaction of terephthalic acid derivs. (II; X, Y = OR1 , OR2 Cl, Br, iodo, NHR; R-R2 = independently H or C1-6 alkyl) with formaldehyde or its equivalent (trioxane or paraformaldehyde) or oleum and (b) addition of an alc. R3-OH to the reaction of step (a). The 5-alkoxycarbonylphthtalides are useful in syntheses of the well-known antidepressants citalopram and escitalopram. Thus, oleum (20-25% SO3, 160 L) was charged into a glass reactor (400 L) and under stirring di-Me terephthalate (90.7 kg) was added to the reactor, followed by adding paraformaldehyde (18.6 kg). The reaction mixture was agitated at 125° for 5 h, cooled to 70°, and added to a reactor containing ethanol (620 L) at ambient temperature about 20°. The mixture was heated at 85-93° for 1.5 h and then cooled to approximated 80° before ice (240 kg) was added. After stirring overnight the mixture was cooled to 15° and the precipitate was filtered off and washed with water (150 L). The crude product was added to a stirred mixture of water (250 L) and to this slurry was added NaOH (27.7%, approximated 250 L) to a pH about 4. The precipitate was filtered off and washed with water (500 L) and dried to give 83% 5-ethoxycarbonylphtalide.

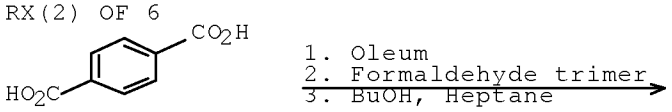
RX(1) OF 6



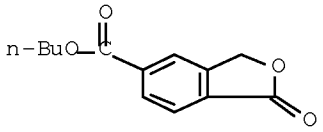
(step 1)

NOTE: pilot plant, scalable, paraformaldehyde was used
CON: STAGE(1) room temperature; 5 hours, 125 deg C;
125 deg C -> 70 deg C
STAGE(2) 1.5 hours, 85 - 93 deg C; 93 deg C -> 80 deg C

RX(2) OF 6



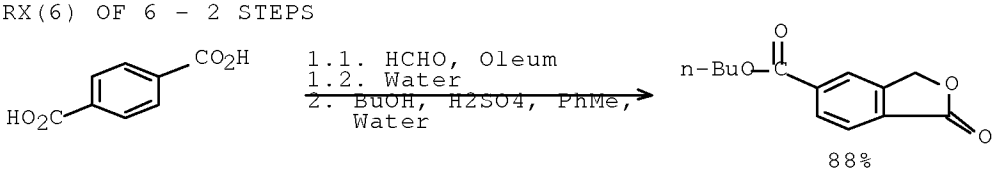
(step 1)



54%

NOTE: optimization study, thermal
CON: STAGE(1) room temperature -> 60 deg C; 30 minutes; 60 minutes, 100 deg C; 100 deg C -> 30 deg C
STAGE(2) 1.5 hours, 130 - 135 deg C; 4 hours, 155 deg C; 155 deg C -> 40 deg C

RX(6) OF 6 - 2 STEPS



88%

NOTE: 1) paraformaldehyde was used, thermal
CON: STEP(1.1) room temperature -> 150 deg C; - 2 hour, 150 deg C; 4 hours, 150 deg C; 150 deg C -> 90 deg C
STEP(1.2) <100 deg C
STEP(2) room temperature -> 85 deg C

L25 ANSWER 4 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 134:326395 CASREACT Full-text
TITLE: Regioselective preparation of 5-carboxyphthalide by the cyclocondensation of terephthalic acid with paraformaldehyde in oleum
INVENTOR(S): Petersen, Hans; Dahlberg, Nielsen Poul
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 9 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032642	A1	20010510	WO 2000-DK585	20001019

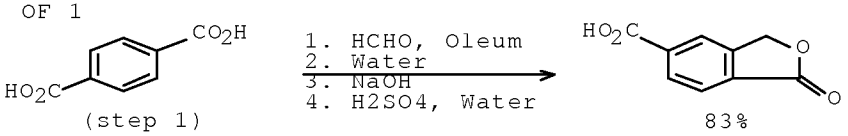
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2389379	A1	20010510	CA 2000-2389379	20001019
CA 2389379	C	20070410		
US 6403813	B1	20020611	US 2000-692653	20001019
BR 2000015471	A	20020709	BR 2000-15471	20001019
EP 1235819	A1	20020904	EP 2000-969234	20001019
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003513084	T	20030408	JP 2001-534793	20001019
IT 1319251	B1	20030926	IT 2000-MI2342	20001027
MX 2002PA04313	A	20021107	MX 2002-PA4313	20020430
US 20020165403	A1	20021107	US 2002-140361	20020506
US 6888009	B2	20050503		
IN 2002CN00774	A	20050520	IN 2002-CN774	20020524
HK 1052702	A1	20050923	HK 2003-104993	20030710
PRIORITY APPLN. INFO.:			DK 1999-1569	19991101
			US 2000-692653	20001019
			WO 2000-DK585	20001019

AB 5-Carboxyphthalide, a pharmaceutical intermediate, is prepared, on an industrial scale, in very high yield and purity by a the regioselective cyclocondensation of terephthalic acid with paraformaldehyde in the presence of oleum.

RX(1) OF 1



(step 1) 83%

NOTE: paraformaldehyde used

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 11 CASREACT COPYRIGHT 2008 ACS on STN DUPLICATE 5

ACCESSION NUMBER: 135:107244 CASREACT Full-text

TITLE: High-yield process for the preparation of 5-carboxyphthalide by the reaction of terephthalic acid with formaldehyde in the presence of oleum

INVENTOR(S): Dall'Asta, Leone; Casazza, Umberto; Cotticelli, Giovanni

PATENT ASSIGNEE(S): Norpharma S.p.A., Italy

SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1118614	A2	20010725	EP 2000-203602	20001017
EP 1118614	A3	20011024		

EP 1118614	B1	20020619			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
IT 2000MI0050	A1	20010718	IT 2000-MI50	20000118	
IT 1317729	B1	20030715			
AT 219489	T	20020715	AT 2000-203602	20001017	
PT 1118614	T	20021129	PT 2000-203602	20001017	
ES 2178626	T3	20030101	ES 2000-203602	20001017	
JP 2001206881	A	20010731	JP 2000-372224	20001207	
CA 2397497	A1	20010726	CA 2001-2397497	20010117	
WO 2001053284	A1	20010726	WO 2001-EP617	20010117	
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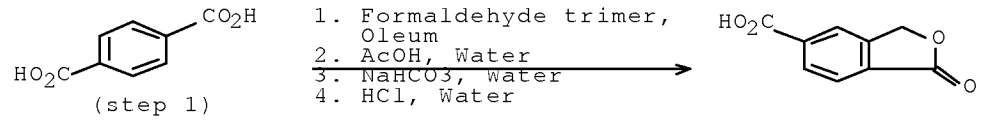
RW: GH, GM, KE, LS, MW, MZ, SD, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
AU 2001026798	A	20010731	AU 2001-26798	20010117	
AU 779581	B2	20050127			
EP 1187822	A1	20020320	EP 2001-901181	20010117	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
BR 2001007853	A	20021029	BR 2001-7853	20010117	
HU 2002004187	A2	20030328	HU 2002-4187	20010117	
HU 2002004187	A3	20050530			
RO 121737	B1	20080328	RO 2002-989	20010117	
HK 1042290	A1	20030718	HK 2002-100631	20020125	
ZA 2002005475	A	20031010	ZA 2002-5475	20020709	
IN 2002KN00905	A	20050701	IN 2002-KN905	20020709	
BG 106925	A	20040130	BG 2002-106925	20020716	
MX 2002PA07031	A	20040906	MX 2002-PA7031	20020718	
US 20030009038	A1	20030109	US 2002-227038	20020823	
US 6703516	B2	20040309			
US 20040171851	A1	20040902	US 2004-796336	20040308	
PRIORITY APPLN. INFO.:			IT 2000-MI50	20000118	
			US 2000-690301	20001017	
			WO 2001-EP617	20010117	
			US 2002-227038	20020823	

AB A process for the preparation of 5-carboxyphthalide comprises adding terephthalic acid to fuming sulfuric acid (i.e., oleum) containing ≥20% of SO3, then adding formaldehyde to the mixture, heating it at 120-145°, and isolating 5-carboxyphthalide.

RX(1) OF 1



L25 ANSWER 6 OF 11 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:156327 CASREACT Full-text
TITLE: Methods for the preparation of rhodamine for use in peptide synthesis
INVENTOR(S): Damoiseaux, Robert D.; Harris, Jennifer L.
PATENT ASSIGNEE(S): IRM LLC, Bermuda
SOURCE: PCT Int. Appl., 29 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

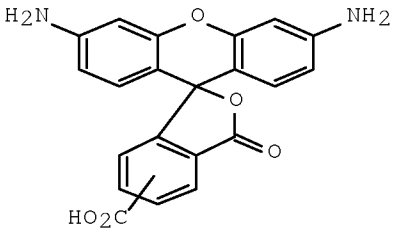
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005007678	A2	20050127	WO 2004-US22775	20040714
WO 2005007678	A3	20050407		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 20050113584	A1	20050526	US 2004-891826	20040714

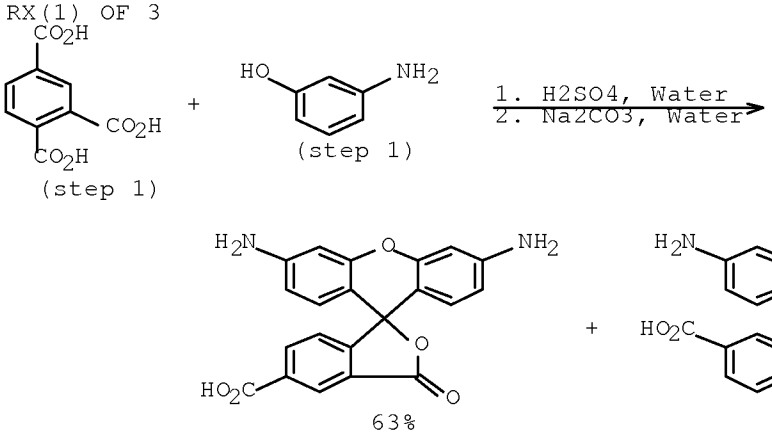
PRIORITY APPLN. INFO.: US 2003-487331P 20030714
OTHER SOURCE(S): MARPAT 142:156327
GI



I

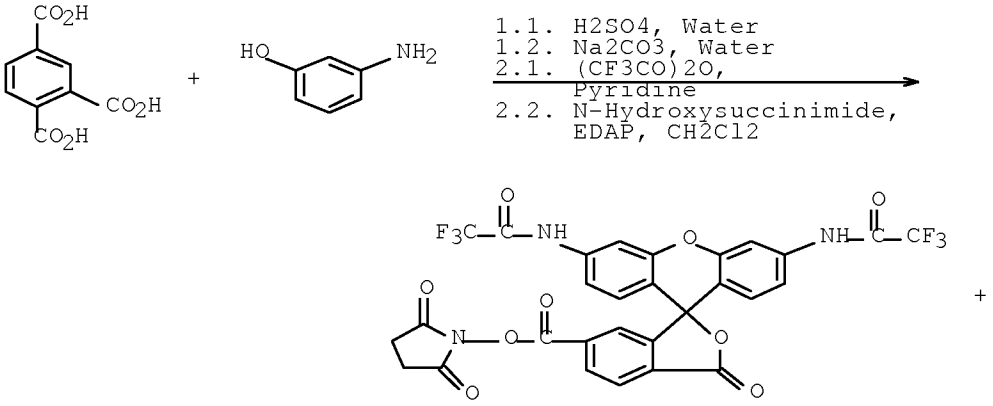
AB The invention relates to a method for preparing rhodamine (I) on a solid support and, in particular, methods for the economical preparation of rhodamine NHS ester. The attachment of rhodamine NHS ester to a solid support and use of the rhodamine free amines as attachment points for peptides is especially attractive in peptide chemical and in screening assays for protease activity. Thus, stirring a mixture of 1,2,4-benzenetricarboxylic acid and 3-aminophenol in H2SO4 at 180℃ for 6 h afforded 63% rhodamine of about 90% purity.

RX(1) OF 3

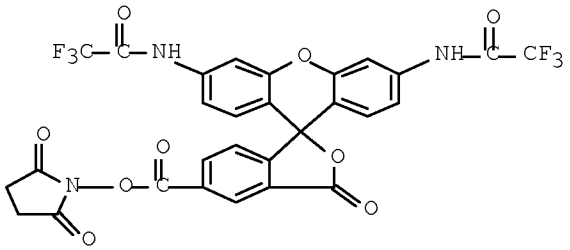


NOTE: thermal
CON: STAGE(1) room temperature; room temperature -> 180 deg C; 6 hours, 180 deg C; cooled
STAGE(2) neutralized

RX(3) OF 3 - 2 STEPS



RX(3) OF 3 - 2 STEPS

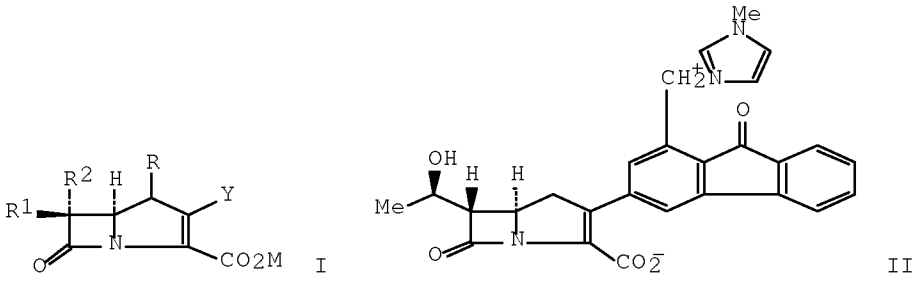


NOTE: 1) thermal, 2) combined yield of 14%
CON: STEP(1.1) room temperature; room temperature -> 180 deg C;
6 hours, 180 deg C; cooled
STEP(1.2) neutralized
STEP(2.1) room temperature; overnight, room temperature
STEP(2.2) room temperature; 35 minutes, room temperature

L25 ANSWER 7 OF 11 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 116:59077 CASREACT Full-text
TITLE: Preparation of 2-(9-fluorenonyl)carbapenem antibacterial agents
INVENTOR(S): Greenlee, Mark L.; DiNinno, Frank P.; Cama, Lovji D.; Heck, James V.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 85 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5034384	A	19910723	US 1990-561547	19900801
EP 472306	A1	19920226	EP 1991-306955	19910730
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 9103655	A	19920202	FI 1991-3655	19910731
NO 9102980	A	19920203	NO 1991-2980	19910731
AU 9181517	A	19920206	AU 1991-81517	19910731
AU 642518	B2	19931021		
ZA 9106019	A	19920429	ZA 1991-6019	19910731
JP 05105679	A	19930427	JP 1991-280913	19910731
JP 2509771	B2	19960626		
CA 2048269	A1	19920202	CA 1991-2048269	19910801
US 5356889	A	19941018	US 1992-966969	19921026
PRIORITY APPLN. INFO.:			US 1990-561547	19900801
			US 1990-594808	19901009

OTHER SOURCE(S): MARPAT 116:59077
GI

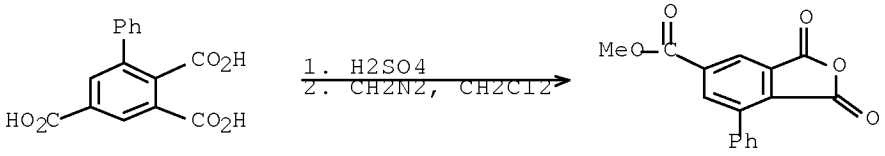


I II

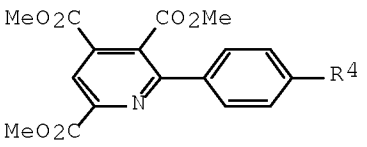
AB The title compds. [I; M = H, ester residue, alkali metal cation, neg. charge, etc.; R = H, Me; R1, R2 = H, Me, Et, CH2OH, MeCH(OH), etc.; Y = 9-fluorenon-2- or -3-yl optionally substituted by, e.g., 1-methylimidazolium-3-ylmethyl, 4-amino-1,2,4-triazolium-1-ylmethyl, 2-aminopyridinium-1-ylmethyl, etc.] were prepared as antibiotics (no data). Thus, 4-nitrobenzyl (5R,6S)-2-oxo-6-[(1R)-hydroxyethyl]carbapenem-3- carboxylate was condensed with 3-trimethylstannyl-1-hydroxymethyl-9- fluorenone (preparation given) and the product condensed with 1-methylimidazole to give, after deprotection, title compound II.

RX(4) OF 232

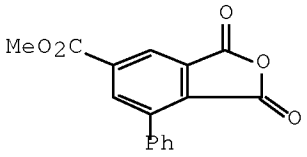
RX(48) OF 232 - 2 STEPS



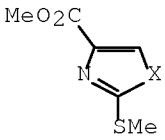
L25 ANSWER 8 OF 11 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 95:7151 CASREACT Full-text
TITLE: New 4-amino-2-azabutadienes and 1-aminobutadienes: synthesis from pyridines, benzenes, and azoles
AUTHOR(S): Gompper, Rudolf; Heinemann, Ulrich
CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, D-8000/2, Fed. Rep. Ger.
SOURCE: Angewandte Chemie (1981), 93(3), 297-8
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



III



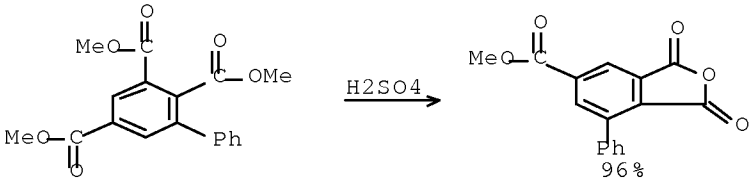
IV



VI, X=O
VII, X=S
VIII, X=NR5

AB R1CH2N:CR2R3 [R1 = CO2Me, cyano; R2 = H, Me; R3 = 4-R4C6H4 (R4 = H, Cl, Me, Me2N), SMe, NMe2] heated with HC(OEt)2NMe2 [or [Me2NCHCl]+ Cl- for MeO2CCH2N:CHNMe2] gave 35-87% Me2NCH:CR1N:CR2R3 (I). A mixture of MeO2CCH2CH:CHPh and MeO2CCH:CHCH2Ph similarly gave 71% Me2NCH:C(CO2Me)CH:CHPh (II). I (R1 = CO2Me, R2 = H, R3 = H, Cl, Me) cyclized with MeO2CC.tplbond.CCO2Me to give 15-41% pyridines III, and II gave 35% 2,3,5-(MeO2C)3C6H2Ph, which gave 96% anhydride IV with concentrated H2SO4. Boiling II (R1 = CO2Me, R2 = R3 = SMe) (V) in THF-dilute HCl gave 86% oxazole VI, whereas passing HCl through V in THF at 20°, then H2S while heating the mixture gave 85% thiazole VII. Heating V with R5NH2.HCl (R5 = Ph, CH2Ph) in dioxane-DMF gave 22-38% imidazoles VIII.

RX(13) OF 24



11 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):9-11

L25 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:534492 CAPLUS Full-text
DOCUMENT NUMBER: 145:29562
TITLE: Water-thinned polyester-based resin compositions for coating of cans, and coated metal sheets
INVENTOR(S): Tajika, Hiroshi
PATENT ASSIGNEE(S): Toyobo Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006143891	A	20060608	JP 2004-335972	20041119
PRIORITY APPLN. INFO.:			JP 2004-335972	20041119

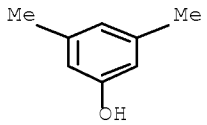
AB The resin compns. contain polyesters (A) (acid value 150-800 equiv/106 g, Mn 5,000-100,000) consisting of polycarboxylic acid components containing 70-100 mol% aromatic dicarboxylic acids and 0-30 mol% other polycarboxylic acids and polyol components containing 40-100 mol% (in total) 2-ethyl-2-butyl-1,3-propanediol and 2-methyl-1,3-propanediol, 1,4-butanediol, and/or 1,4-cyclohexanedimethanol and 0-60 mol% other polyols, resol-type phenolic resins (B), basic compds. (C), and H2O. Thus, a water-thinned coating composition containing 85 parts of 30:69:4:20:55:25 (by mol) terephthalic acid-isophthalic acid-trimellitic anhydride-2-ethyl-2-butyl-1,3-propanediol-1,4-butanediol-1,4-cyclohexanedimethanol copolymer (Mn 15,000, acid value 230 equiv/106 g), 15 parts resol-type m-cresol-formaldehyde copolymer, and 2.1 parts N,N-dimethylethanolamine was applied on an Al sheet (5052) and baked to give a coated test piece showing good curability, workability, overbake resistance, retort resistance, acid resistance, and dent resistance,.

IT 25086-35-5P, Formaldehyde-3,5-xylenol copolymer
25086-36-6P, m-Cresol-formaldehyde copolymer
RL: IMF (Industrial manufacture); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(resol, crosslinking agent; water-thinned coatings containing polyesters, resols, and basic compds. for coated metal cans with good workability, overbake resistance, and retort resistance)

RN 25086-35-5 CAPLUS
CN Formaldehyde, polymer with 3,5-dimethylphenol (CA INDEX NAME)

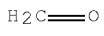
CM 1

CRN 108-68-9
CMF C8 H10 O



CM 2

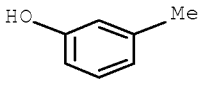
CRN 50-00-0
CMF C H2 O



RN 25086-36-6 CAPLUS
CN Formaldehyde, polymer with 3-methylphenol (CA INDEX NAME)

CM 1

CRN 108-39-4
CMF C7 H8 O



CM 2

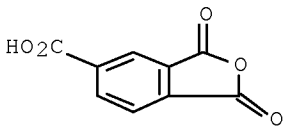
CRN 50-00-0
CMF C H2 O

IT 889651-66-5P 889651-68-7P 889651-70-1P
889651-72-3P
RL: IMF (Industrial manufacture); RCT (Reactant); TEM
(Technical or engineered material use); PREP (Preparation);
RACT (Reactant or reagent); USES (Uses)
(water-thinned coatings containing polyesters, resols, and basic compds. for coated metal cans with good workability, overbake resistance, and retort resistance)

RN 889651-66-5 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol and 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid (9CI) (CA INDEX NAME)

CM 1

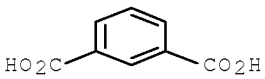
CRN 552-30-7
CMF C9 H4 O5



CM 2

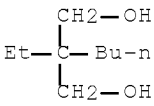
CRN 121-91-5

CMF C8 H6 O4



CM 3

CRN 115-84-4
CMF C9 H20 O2

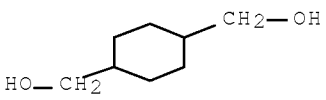


CM 4

CRN 110-63-4
CMF C4 H10 O2

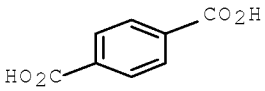
CM 5

CRN 105-08-8
CMF C8 H16 O2



CM 6

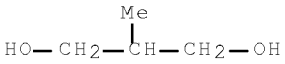
CRN 100-21-0
CMF C8 H6 O4



RN 889651-68-7 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate) and 2-methyl-1,3-propanediol (9CI) (CA INDEX NAME)

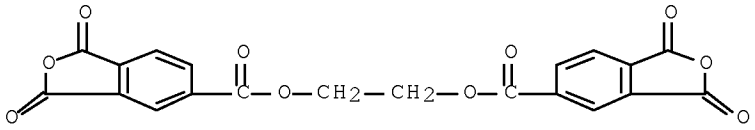
CM 1

CRN 2163-42-0
CMF C4 H10 O2



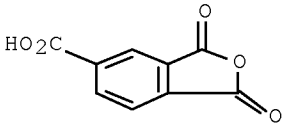
CM 2

CRN 1732-96-3
CMF C20 H10 O10



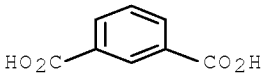
CM 3

CRN 552-30-7
CMF C9 H4 O5



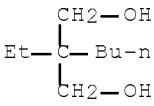
CM 4

CRN 121-91-5
CMF C8 H6 O4



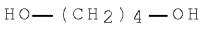
CM 5

CRN 115-84-4
CMF C9 H20 O2



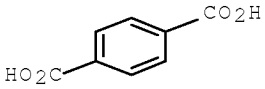
CM 6

CRN 110-63-4
CMF C4 H10 O2



CM 7

CRN 100-21-0
CMF C8 H6 O4

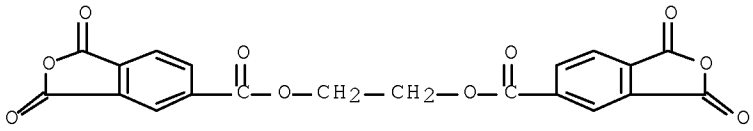


RN 889651-70-1 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, decanedioic acid, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediol and 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate)

(9CI) (CA INDEX NAME)

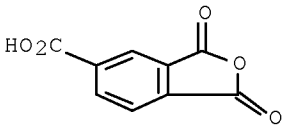
CM 1

CRN 1732-96-3
CMF C20 H10 O10



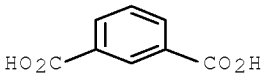
CM 2

CRN 552-30-7
CMF C9 H4 O5



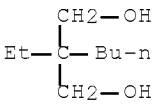
CM 3

CRN 121-91-5
CMF C8 H6 O4



CM 4

CRN 115-84-4
CMF C9 H20 O2

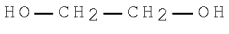


CM 5

CRN 111-20-6
CMF C10 H18 O4

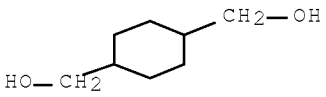
CM 6

CRN 107-21-1
CMF C2 H6 O2



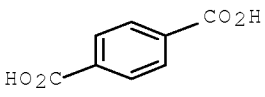
CM 7

CRN 105-08-8
CMF C8 H16 O2



CM 8

CRN 100-21-0
CMF C8 H6 O4

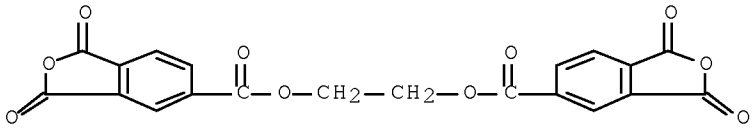


RN 889651-72-3 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic

acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate) and 4-hydroxy-γ-(4-hydroxyphenyl)-γ-methylbenzenebutanoic acid (9CI) (CA INDEX NAME)

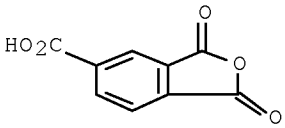
CM 1

CRN 1732-96-3
CMF C20 H10 O10



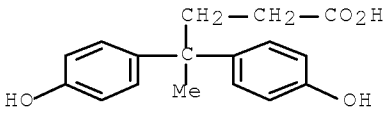
CM 2

CRN 552-30-7
CMF C9 H4 O5



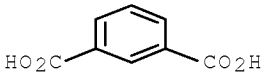
CM 3

CRN 126-00-1
CMF C17 H18 O4



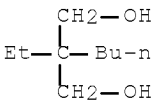
CM 4

CRN 121-91-5
CMF C8 H6 O4



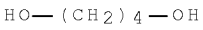
CM 5

CRN 115-84-4
CMF C9 H20 O2



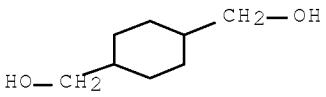
CM 6

CRN 110-63-4
CMF C4 H10 O2



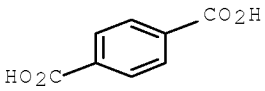
CM 7

CRN 105-08-8
CMF C8 H16 O2



CM 8

CRN 100-21-0
CMF C8 H6 O4



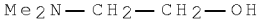
IT 889651-75-6P 889651-78-9P 889651-81-4P
889651-83-6P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(water-thinned coatings containing polyesters, resols, and basic compds. for coated metal cans with good workability, overbake resistance, and retort resistance)

RN 889651-75-6 CAPLUS

CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, formaldehyde and 3-methylphenol, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0
CMF C4 H11 N O

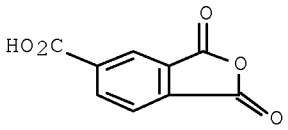


CM 2

CRN 889651-74-5
CMF (C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H6 O4 . C8 H6 O4 . C7 H8 O . C4 H10 O2 . C H2 O)x
CCI PMS

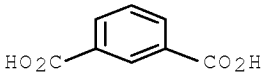
CM 3

CRN 552-30-7
CMF C9 H4 O5



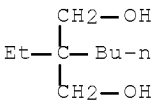
CM 4

CRN 121-91-5
CMF C8 H6 O4



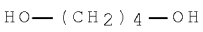
CM 5

CRN 115-84-4
CMF C9 H20 O2



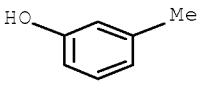
CM 6

CRN 110-63-4
CMF C4 H10 O2



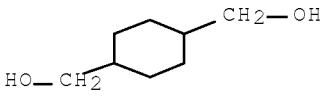
CM 7

CRN 108-39-4
CMF C7 H8 O



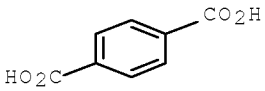
CM 8

CRN 105-08-8
CMF C8 H16 O2



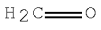
CM 9

CRN 100-21-0
CMF C8 H6 O4



CM 10

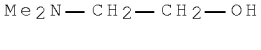
CRN 50-00-0
CMF C H2 O



RN 889651-78-9 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate), formaldehyde, 3-methylphenol and 2-methyl-1,3-propanediol, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0
CMF C4 H11 N O



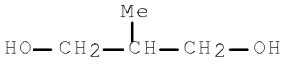
CM 2

CRN 889651-77-8
CMF (C20 H10 O10 . C9 H20 O2 . C9 H4 O5 . C8 H6 O4 . C8 H6 O4 . C7 H8 O . C4 H10 O2 . C4 H10 O2 . C H2 O)x
CCI PMS

CM 3

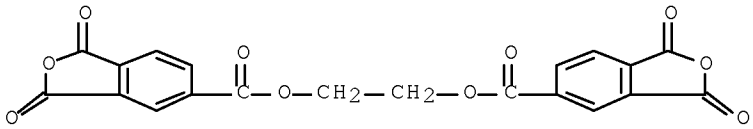
CRN 2163-42-0

CMF C4 H10 O2



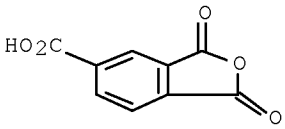
CM 4

CRN 1732-96-3
CMF C20 H10 O10



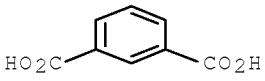
CM 5

CRN 552-30-7
CMF C9 H4 O5



CM 6

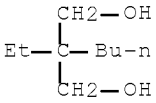
CRN 121-91-5
CMF C8 H6 O4



CM 7

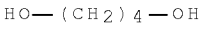
CRN 115-84-4

CMF C9 H20 O2



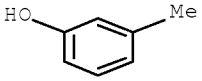
CM 8

CRN 110-63-4
CMF C4 H10 O2



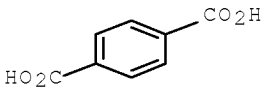
CM 9

CRN 108-39-4
CMF C7 H8 O



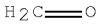
CM 10

CRN 100-21-0
CMF C8 H6 O4



CM 11

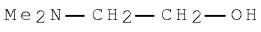
CRN 50-00-0
CMF C H2 O



RN 889651-81-4 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, decanedioic acid, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 3,5-dimethylphenol, 1,2-ethanediol, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate) and formaldehyde, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0
CMF C4 H11 N O

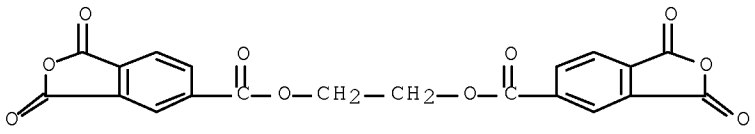


CM 2

CRN 889651-80-3
CMF (C20 H10 O10 . C10 H18 O4 . C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H10 O . C8 H6 O4 . C8 H6 O4 . C2 H6 O2 . C H2 O)x
CCI PMS

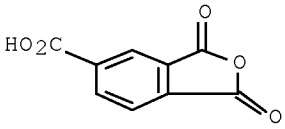
CM 3

CRN 1732-96-3
CMF C20 H10 O10



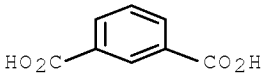
CM 4

CRN 552-30-7
CMF C9 H4 O5



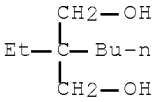
CM 5

CRN 121-91-5
CMF C8 H6 O4



CM 6

CRN 115-84-4
CMF C9 H20 O2

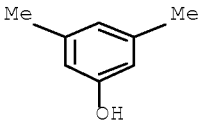


CM 7

CRN 111-20-6
CMF C10 H18 O4

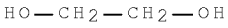
CM 8

CRN 108-68-9
CMF C8 H10 O



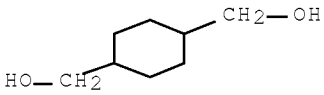
CM 9

CRN 107-21-1
CMF C2 H6 O2



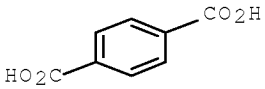
CM 10

CRN 105-08-8
CMF C8 H16 O2



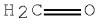
CM 11

CRN 100-21-0
CMF C8 H6 O4



CM 12

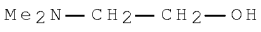
CRN 50-00-0
CMF C H2 O



RN 889651-83-6 CAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-benzenedicarboxylic acid, 1,4-butanediol, 2-butyl-2-ethyl-1,3-propanediol, 1,4-cyclohexanedimethanol, 1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylic acid, 3,5-dimethylphenol, 1,2-ethanediyl bis(1,3-dihydro-1,3-dioxo-5-isobenzofurancarboxylate), formaldehyde and 4-hydroxy-γ-(4-hydroxyphenyl)-γ-methylbenzenebutanoic acid, compd. with 2-(dimethylamino)ethanol (9CI) (CA INDEX NAME)

CM 1

CRN 108-01-0
CMF C4 H11 N O

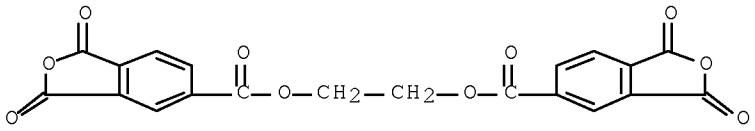


CM 2

CRN 889651-82-5
CMF (C20 H10 O10 . C17 H18 O4 . C9 H20 O2 . C9 H4 O5 . C8 H16 O2 . C8 H10 O . C8 H6 O4 . C8 H6 O4 . C4 H10 O2 . C H2 O)x
CCI PMS

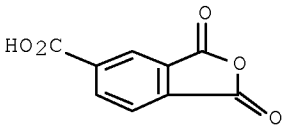
CM 3

CRN 1732-96-3
CMF C20 H10 O10



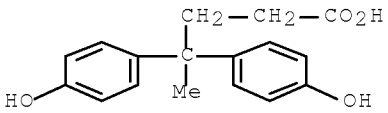
CM 4

CRN 552-30-7
CMF C9 H4 O5



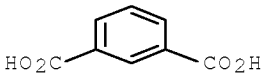
CM 5

CRN 126-00-1
CMF C17 H18 O4



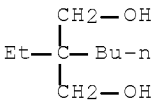
CM 6

CRN 121-91-5
CMF C8 H6 O4



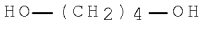
CM 7

CRN 115-84-4
CMF C9 H20 O2



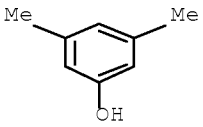
CM 8

CRN 110-63-4
CMF C4 H10 O2



CM 9

CRN 108-68-9
CMF C8 H10 O



CM 10

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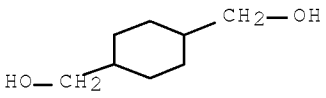
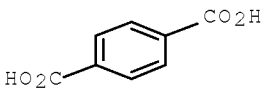


CM 11

CRN 100-21-0
CMF C8 H6 O4



CM 12

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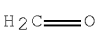
CMF C H2 O



L25 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:338514 CAPLUS Full-text
DOCUMENT NUMBER: 134:326396
TITLE: Method for the preparation of 5-carboxyphthalide from terephthalic acid and trioxane or paraformaldehyde

INVENTOR(S): Petersen, Hans
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 8 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032643	A1	20010510	WO 2000-DK606	20001101

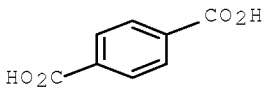
W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DK 1999-1568 A 19991101
OTHER SOURCE(S): CASREACT 134:326396

AB 5-Carboxyphthalide, useful as an antidepressant intermediate, is prepared in high yield and selectivity by the cyclocondensation reaction of terephthalic acid with trioxane or paraformaldehyde in the presence of a Lewis acid (e.g., ZnCl2) or a mineral acid (e.g., polyphosphoric acid).

IT 100-21-0, Terephthalic acid, reactions 110-88-3, 1,3,5-Trioxane, reactions 30525-89-4, Paraformaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(method for the preparation of 5-carboxyphthalide from terephthalic acid and trioxane or paraformaldehyde)

RN 100-21-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid (CA INDEX NAME)

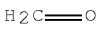


RN 110-88-3 CAPLUS
CN 1,3,5-Trioxane (CA INDEX NAME)

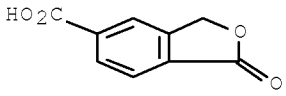
RN 30525-89-4 CAPLUS
CN Paraformaldehyde (CA INDEX NAME)

CM 1

CRN 50-00-0
CMF C H2 O

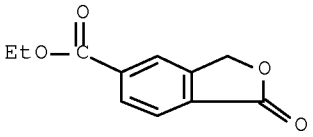


IT 4792-29-4P, 5-Carboxyphthalide
RL: SPN (Synthetic preparation); PREP (Preparation)
(method for the preparation of 5-carboxyphthalide from terephthalic acid and
trioxane or paraformaldehyde)
RN 4792-29-4 CAPLUS
CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo- (CA INDEX NAME)

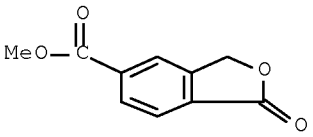


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

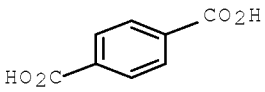
L25 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:403627 CAPLUS Full-text
DOCUMENT NUMBER: 73:3627
ORIGINAL REFERENCE NO.: 73:613a,616a
TITLE: Reaction of terephthalic acid with formaldehyde in sulfur trioxide media
AUTHOR(S): Forney, LeRoy S.
CORPORATE SOURCE: Res. and Develop. Lab., Mobil Chem. Co., Edison, NJ, USA
SOURCE: Journal of Organic Chemistry (1970), 35(5), 1695-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title acid is treated with H2CO in SO3 at 120-30° to give 5-carboxyphthalide (I); 2-hydroxymethylterephthalic acid is prepared by the saponification of I. Excess H2CO gives p-HO2CC6H4CO2CH2CO2H.
IT 23405-31-4P 23405-32-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23405-31-4 CAPLUS
CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo-, ethyl ester (CA INDEX NAME)



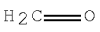
RN 23405-32-5 CAPLUS
CN 5-Isobenzofurancarboxylic acid, 1,3-dihydro-1-oxo-, methyl ester (CA INDEX NAME)



IT 100-21-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with formaldehyde)
RN 100-21-0 CAPLUS
CN 1,4-Benzenedicarboxylic acid (CA INDEX NAME)



IT 50-00-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(with terephthalic acid)
RN 50-00-0 CAPLUS
CN Formaldehyde (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 14:59:19 ON 29 SEP 2008)

FILE 'CASREACT' ENTERED AT 14:59:34 ON 29 SEP 2008

FILE 'REGISTRY' ENTERED AT 14:59:40 ON 29 SEP 2008
L1 STR

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     FILE 'REGISTRY' ENTERED AT 15:03:54 ON 29 SEP 2008
                E FUMING SULFURIC/CN
L2              1 SEA ABB=ON  PLU=ON  "FUMING SULFURIC ACID"/CN
                D SCA

     FILE 'CASREACT' ENTERED AT 15:04:30 ON 29 SEP 2008
L3              STR L1
L4              1 SEA SSS SAM L3 (     2 REACTIONS)
L5              8 SEA SSS FUL L3 (    13 REACTIONS)

     FILE 'REGISTRY' ENTERED AT 15:06:14 ON 29 SEP 2008
L6              STR L3
L7             50 SEA SSS SAM L6
L8          12145 SEA SSS FUL L6

     FILE 'REGISTRY' ENTERED AT 15:07:46 ON 29 SEP 2008
                E TEREPHTHALIC ACID/CN
L9              1 SEA ABB=ON  PLU=ON  "TEREPHTHALIC ACID"/CN
                D SCA
                D

     FILE 'REGISTRY' ENTERED AT 15:08:42 ON 29 SEP 2008
L10             STR 100-21-0
L11         27124 SEA FAM FUL L10
L12             1 SEA ABB=ON  PLU=ON  FORMALDEHYDE/CN
L13             1 SEA ABB=ON  PLU=ON  PARAFORMALDEHYDE/CN
L14             1 SEA ABB=ON  PLU=ON  1,3,5-TRIOXANE/CN
L15             3 SEA ABB=ON  PLU=ON  (L12 OR L13 OR L14)
                SEL RN
L16         29207 SEA ABB=ON  PLU=ON  (110-88-3/CRN OR 30525-89-4/CRN OR
                50-00-0/CRN) OR L15

     FILE 'CAPLUS' ENTERED AT 15:10:54 ON 29 SEP 2008
L17            49 SEA ABB=ON  PLU=ON  L11(L)RACT+NT/RL AND L16(L)RACT+NT/RL
L18          5714 SEA ABB=ON  PLU=ON  L8(L)PREP+NT/RL
L19             8 SEA ABB=ON  PLU=ON  L18 AND L17

     FILE 'REGISTRY' ENTERED AT 15:12:05 ON 29 SEP 2008
                SEL RN L2
L20             1 SEA ABB=ON  PLU=ON  L2 OR 8014-95-7/CRN

     FILE 'CAPLUS' ENTERED AT 15:12:48 ON 29 SEP 2008
L21           567 SEA ABB=ON  PLU=ON  L20(L)RACT+NT/RL
L22             3 SEA ABB=ON  PLU=ON  L19 AND L21
L23             3 SEA ABB=ON  PLU=ON  L21 AND L8 AND (L11 OR L16)
L24             8 SEA ABB=ON  PLU=ON  L19 OR L22 OR L23

     FILE 'CASREACT' ENTERED AT 15:14:40 ON 29 SEP 2008
                D QUE L5

     FILE 'CAPLUS' ENTERED AT 15:14:44 ON 29 SEP 2008
                D QUE L24

     FILE 'CASREACT, CAPLUS' ENTERED AT 15:14:50 ON 29 SEP 2008
L25            11 DUP REM L5 L24 (5 DUPLICATES REMOVED)
                     ANSWERS '1-8' FROM FILE CASREACT
                     ANSWERS '9-11' FROM FILE CAPLUS
                D L25 IBIB ABS CRD 1-8
                D L25 IBIB ABS HITSTR 9011
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